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New helium equation of state for pressurized nanobubbles in UO₂ matrix calculated via molecular dynamics simulations

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During storage helium atoms accumulate in spent fuel via alpha-decay. These helium atoms cluster into microscopic bubbles that change the physical properties of spent fuel. To estimate the impact of such bubble, it is essential to possess a good thermodynamical model for helium interacting with the surrounding matrix including states at high pressures and temperatures.

Therefore, molecular dynamics simulations are carried out to establish a new equation of state for helium in nanobubbles embedded in UO₂ matrix. Four bubbles sizes, ranging from 1 to 10 nm, have been investigated for temperatures ranging from 300 to 900 K and helium concentration ranging from 3.2×10^{-2} to 0.39 mol/cm³. From these data, we are able to fit a new equation of state for helium using the Brearley and MacInnes' model. We observe that helium atom is heterogeneously distributed inside the nanobubble with the apparition of a boundary layer of about 1 nm thick at the surface. We also find an upper limit concentration corresponding to 1.6 helium atom per UO₂ vacancy beyond which no more helium atom can be incorporated into the bubble.

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